

Perfluoroheptanoic acid
375-85-9 | DTXSID1037303

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.08

Global applicability domain: Inside

Local applicability domain index: 9.60e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Chloroethanol</div> <div>Measured: 4.30</div> <div>Predicted: 4.07</div>	<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 4.19</div> <div>Predicted: 4.03</div>	<div>Image not found</div> <div>2-Methyl-1-propanol</div> <div>Measured: 3.93</div> <div>Predicted: 3.95</div>
<div>Image not found</div> <div>2-Butanol</div> <div>Measured: 3.85</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>Pyrrolidine</div> <div>Measured: 4.07</div> <div>Predicted: 4.10</div>	